

ORAL PRESENTATION

Open Access

Putting together the pieces: building a reaction-centric electronic lab notebook for mobile devices

Alex Clark

From 9th German Conference on Chemoinformatics
Fulda, Germany. 10-12 November 2013

The presentation will describe 4 years of work creating chemical structure based user interfaces for mobile devices, combined with creation of cloud-hosted web-services for supporting functionality.

A number of products have been created along the way, for drawing structures and reactions, managing collections of data, searching databases, creating publication quality graphics, sharing and collaborating, calculating properties, and model building for drug discovery research.

The focus will be on the assembly of these core technologies to create a fully featured electronic lab notebook (ELN) product for capturing chemical reactions.

While a number of web or mobile products already exist for laboratory notetaking, none of them provide the high level chemistry understanding and sophisticated cheminformatics functionality that will be described. The ability to combine all of the necessary capabilities onto a mobile device such as an iPhone or iPad demonstrates that this new generation of computing platforms is ready to play an important role in the realm of cheminformatics.

Published: 11 March 2014

doi:10.1186/1758-2946-6-S1-O1

Cite this article as: Clark: Putting together the pieces: building a reaction-centric electronic lab notebook for mobile devices. *Journal of Cheminformatics* 2014 **6**(Suppl 1):O1.

Publish with **ChemistryCentral** and every scientist can read your work free of charge

"Open access provides opportunities to our colleagues in other parts of the globe, by allowing anyone to view the content free of charge."

W. Jeffery Hurst, The Hershey Company.

- available free of charge to the entire scientific community
- peer reviewed and published immediately upon acceptance
- cited in PubMed and archived on PubMed Central
- yours — you keep the copyright

Submit your manuscript here:
<http://www.chemistrycentral.com/manuscript/>



ChemistryCentral

Correspondence: aclark.xyz@gmail.com
1900 St. Jacques 302, Montreal H3J2S1, Canada



© 2014 Clark; licensee Chemistry Central Ltd. This is an Open Access article distributed under the terms of the Creative Commons Attribution License (<http://creativecommons.org/licenses/by/2.0/>), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited. The Creative Commons Public Domain Dedication waiver (<http://creativecommons.org/publicdomain/zero/1.0/>) applies to the data made available in this article, unless otherwise stated.